Thermalisation and heat transport in anharmonic chains

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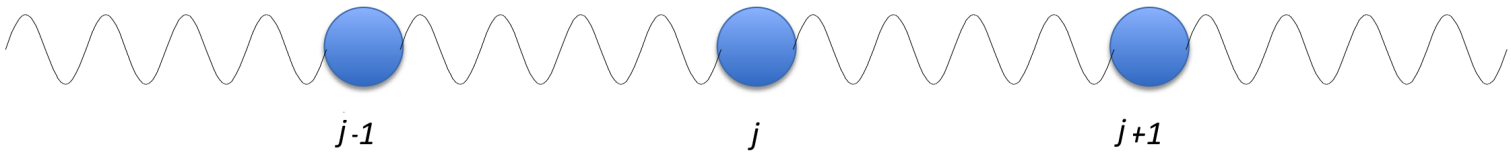


Northumbria University, February 9th, 2022

based on two joint works:
Onorato, et al., PNAS 112, 4208-4213 (2015)
Dematteis, et al., PRL 125 024101 (2020)

About me

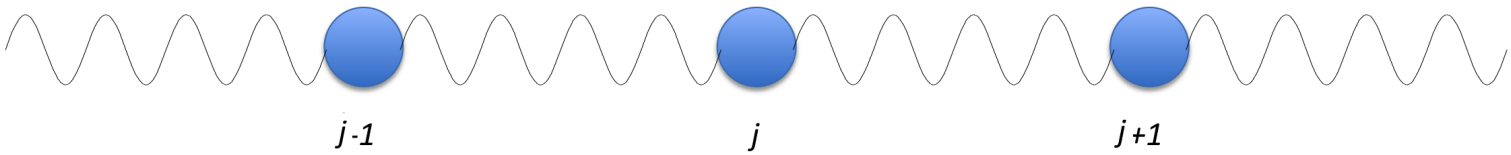
- Background in physics (theoretical physics)
- Main research area is **theory and numerical simulations of quantum fluids**
- In general, I am interested in the dynamics of nonlinear systems where waves/particles/excitations/coherent structures arise and interact (fluids, solids, discrete chains, ...). An example are discrete nonlinear (anharmonic) chains
- Use theory of ODEs/PDEs, Hamiltonian & Lagrangian mechanics, statistical mechanics, nonlinear physics, fluid mechanics, turbulence, quantum mechanics, and numerical simulations

Outline of the talk

- Introduction to the Fermi-Pasta-Ulham(-Tsingou) (FPUT) model for nonlinear (anharmonic) chains
- The wave-wave interaction / wave turbulence approach
- Thermalisation in the α-FPUT system
- Heat transport in the β-FPUT system
- Conclusions and outlooks

The weakly nonlinear chain model (FPUT system)

N equal masses m, at positions q_j with $j = 1, \dots N$, connected by the identical weakly nonlinear springs with their neighbours

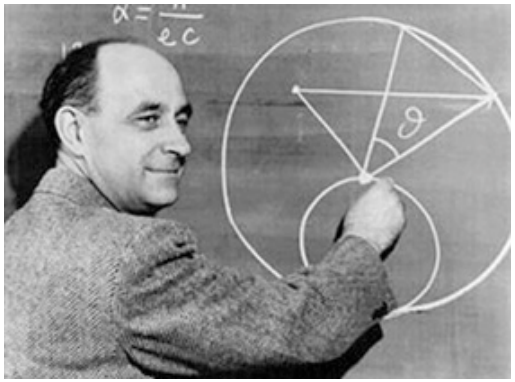


modified Hooke's law $\quad F \simeq -\Delta q(\chi + \alpha \Delta q + \beta \Delta q^2 + \dots)$

The α-FPU system has Hamiltonian in the qs and ps

$$H = \sum_{j=1}^{N} \left[\frac{p_j^2}{2m} + \frac{\chi}{2}(q_j - q_{j+1})^2 + \frac{\alpha}{3}(q_j - q_{j+1})^3 + \frac{\beta}{4}(q_j - q_{j+1})^4 + \dots \right]$$

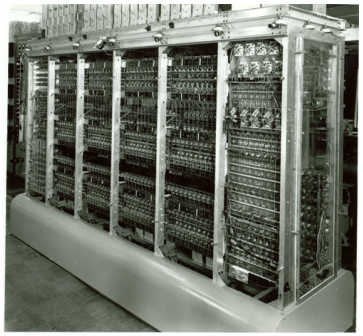
Fermi, Pasta, Ulam (and Tsingou-Menzel) in Los Alamos



Enrico Fermi (1901-1954)

John Pasta (1909-1984)

Stanislaw Ulam (1918-1984)



MANIAC I (1952-1957)

Mary Tsingou-Menzel
(1928-)

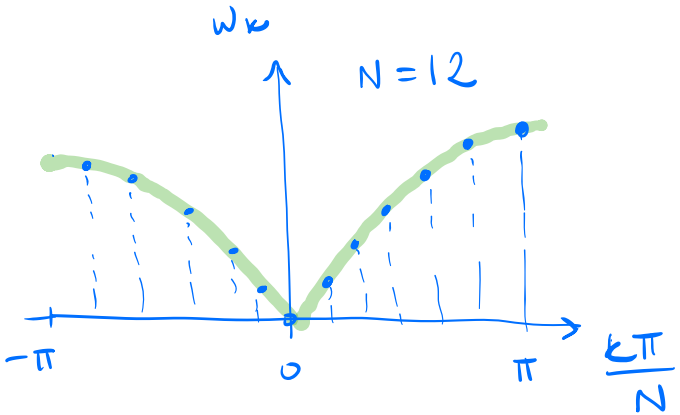
(the story of Mary Tsingou-Menzel is narrated by Thierry Dauxois in the general audience article appeared in Physics Today 56, January 2008)

Solving the linear chain model with normal modes

Assume first to consider the simple linear system, that is the harmonic chain ($\alpha = \beta = 0$). **This is fully solvable!**
Assuming periodic boundary conditions, one introduces the discrete Fourier transform and wave-action variable (normal mode)

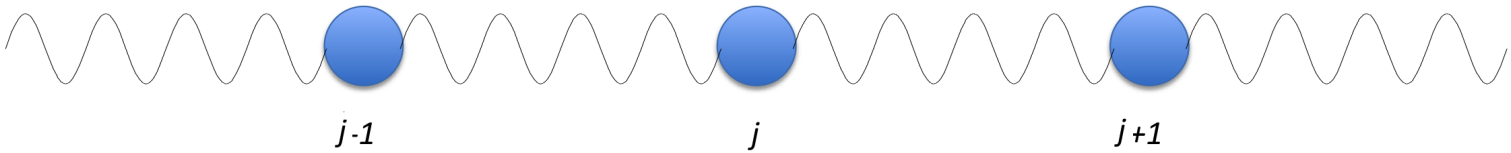
$$Q_k = \frac{1}{N}\sum_{j=0}^{N} q_j\, e^{-i\frac{2\pi}{N}jk}\,,\quad P_k = \dot{Q}_k\,,\quad \omega_k = 2|\sin(\pi k/N)|\,,\quad a_k = \frac{1}{\sqrt{2\,\omega_k}}(P_k - i\omega_k Q_k),$$

$$H = \sum_{j=1}^{N}\left[\frac{p_j^2}{2m} + \frac{\chi}{2}(q_j - q_{j+1})^2\right] \Longrightarrow i\frac{da_k}{dt} = \omega_k a_k,\quad k = -N/2+1,\ldots,N/2$$



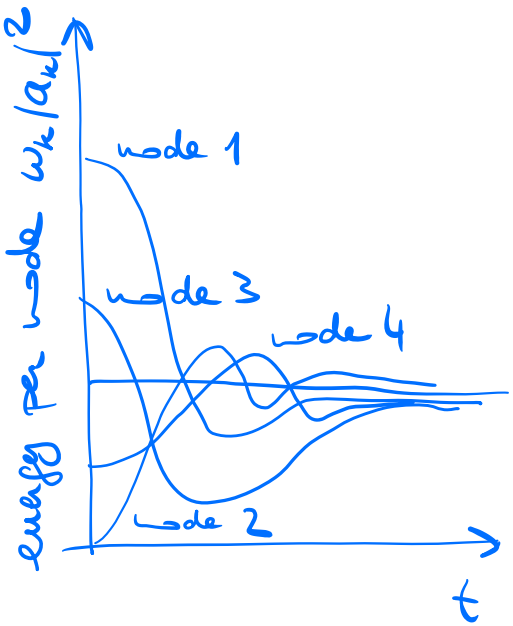
Each mode k **evolves in time independently**,
$a_k(t) = a_k(t_0)e^{-i\omega_k(t-t_0)}$, that is saying that $\omega_k = 2|\sin(\pi k/N)|$ is its angular frequency

The original idea of Fermi



The FPUT model is the simplest toy model to study non-trivial (that is nonlinear) dynamics in solid/crystalline one-dimensional structures

- each mass is an atom and the nonlinear springs mimic the interaction with its two neighbours around the equilibrium
- in time, nonlinear mode interactions will redistribute energy among all the modes of the system
- when (statistical) equipartition of energy has been reached, the system has thermalised, that is it can be described by some non-zero macroscopic temperature
- perturbations on thermal equilibrium can model transfer of heat



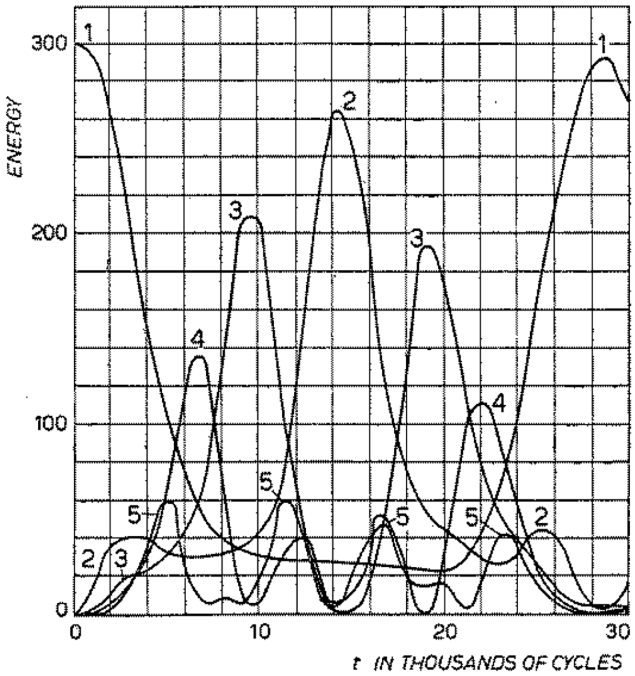
The Los Alamos report

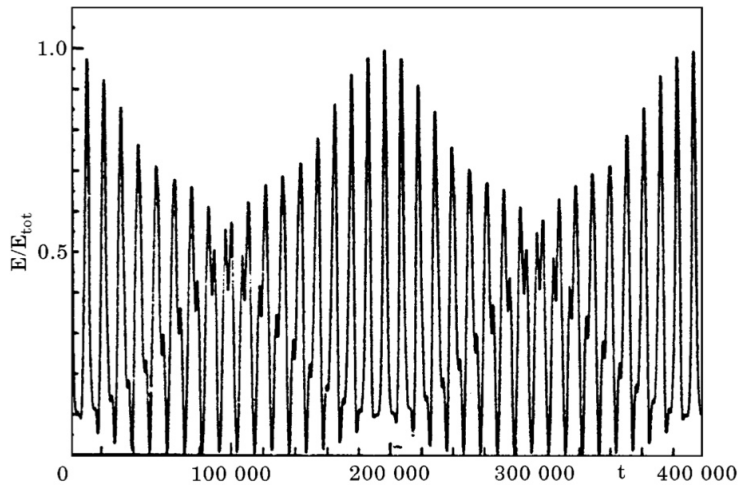
STUDIES OF NON LINEAR PROBLEMS

E. Fermi, J. Pasta, and S. Ulam
Document LA-1940 (May 1955).

A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer MANIAC I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted as a function of time.

The results show very little, if any, tendency toward equipartition of energy among the degrees of freedom.





Tuck & Menzel (1972), The superperiod of the nonlinear weighted string (FPU) problem, Advances in Mathematics, 9(3), 399-407.

Open questions

Several reviews on this topic:

Ford, J. "The Fermi-Pasta-Ulam problem: paradox turns discovery." Physics Reports 213.5 (1992): 271-310; Berman, G. P., and F. M. Izrailev. "The Fermi-Pasta-Ulam problem: fifty years of progress." Chaos (Woodbury, NY) 15.1 (2005): 15104; Carati, A., L. Galgani, and A. Giorgilli. "The Fermi-Pasta-Ulam problem as a challenge for the foundations of physics." Chaos: An Interdisciplinary Journal of Nonlinear Science 15.1 (2005): 015105-015105; Weissert, Thomas P. "The genesis of simulation in dynamics: pursuing the Fermi-Pasta-Ulam problem." Springer-Verlag New York, Inc., 1999; Gallavotti, G., ed. "The Fermi-Pasta-Ulam problem: a status report." Vol. 728. Springer, 2008.

- Does the system thermalise for arbitrary small nonlinearity?
- What is the time-scale of thermalisation for finite N?
- What is the thermalisation time scale in the thermodynamic limit $N \to \infty$?
- What are the transport properties of perturbations over the equilibrium?

The wave-wave interaction approach

Inspired by the wave turbulence theory which may be applied to any weakly nonlinear dispersive system like waves in optics, plasma, ocean, Bose-Einstein condensates [Wave Turbulence, Nazarenko (2011)]

- The (long time) efficient energy transfer in the system goes only trough exact resonant n-wave interaction processes satisfying

$$k_1 \pm k_2 \pm .... \pm k_n = 0$$
$$\omega(k_1) \pm \omega(k_2) \pm ... \pm \omega(k_n) = 0$$

- The long time usually scales as ϵ^{η}, given ϵ the small nonlinear parameter, and η depends on the nonlinearity

The interaction representation

- for instance in a swing one has to push at the right resonant frequency in order to be efficient
- the same idea applies to normal modes where the nonlinear interactions are seen like a forcing term

Introduce the following rotation $a'_k(t) = a_k(t)e^{i\omega_k t}$, then for α-FPUT

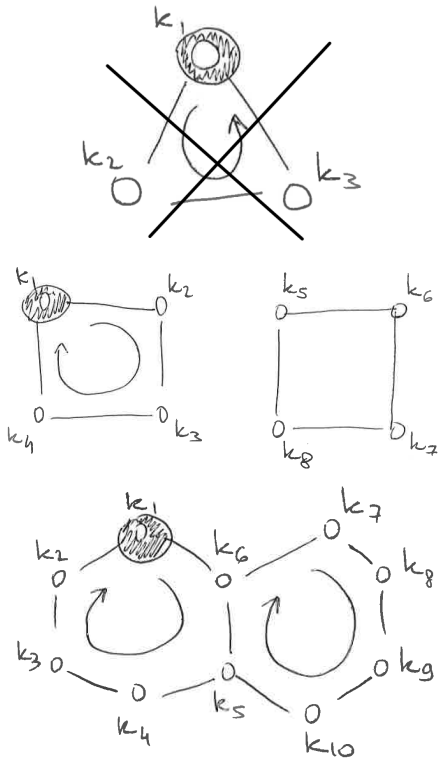
$$i\frac{da'_{k_1}}{dt} = \epsilon \sum_{k_2,k_3} V_{1,2,3}\left(a'_{k_2}a'_{k_3}e^{i\Delta\Omega^{(1)}t}\delta_{k_1,k_2+k_3} + 2\,a'^{*}_{k_2}a'_{k_3}e^{i\Delta\Omega^{(2)}t}\delta_{k_1,k_3-k_2} \right.$$
$$\left. + a'^{*}_{k_2}a'^{*}_{k_3}e^{i\Delta\Omega^{(3)}t}\delta_{k_1,-k_2-k_3}\right) ,$$

$$\begin{aligned}
&\#1 \text{ term:} \quad k_1 - k_2 - k_3\,, \quad \Delta\Omega^{(1)} = \omega_{k_1} - \omega_{k_2} - \omega_{k_3} \\
&\#2 \text{ term:} \quad k_1 + k_2 - k_3\,, \quad \Delta\Omega^{(2)} = \omega_{k_1} + \omega_{k_2} - \omega_{k_3} \\
&\#3 \text{ term:} \quad k_1 + k_2 + k_3\,, \quad \Delta\Omega^{(3)} = \omega_{k_1} + \omega_{k_2} + \omega_{k_3}
\end{aligned}$$

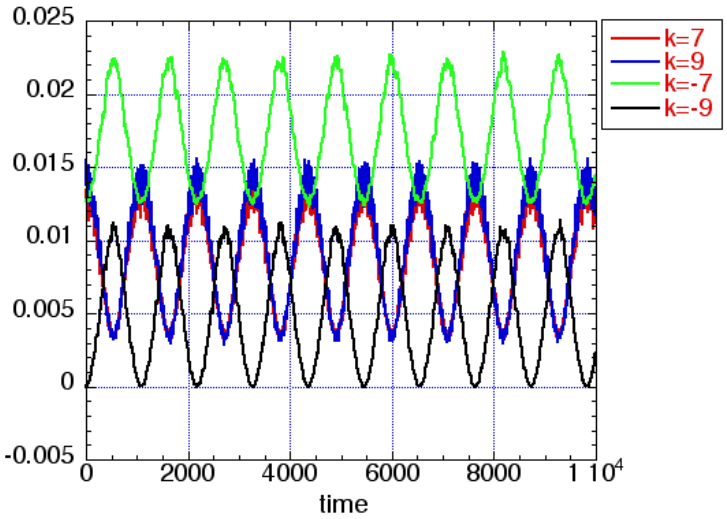
Thermalisation timescale t_{eq} for α-FPUT [PNAS 2015]

$$\begin{aligned} &k_1 \pm k_2 \pm .... \pm k_n = 0 \\ &\omega(k_1) \pm \omega(k_2) \pm ... \pm \omega(k_n) = 0 \end{aligned} \quad \text{, for FPUT} \quad \begin{aligned} &k = -N/2+1, \dots, N/2 \\ &\omega(k) = 2|\sin(\pi k/N)| \end{aligned}$$

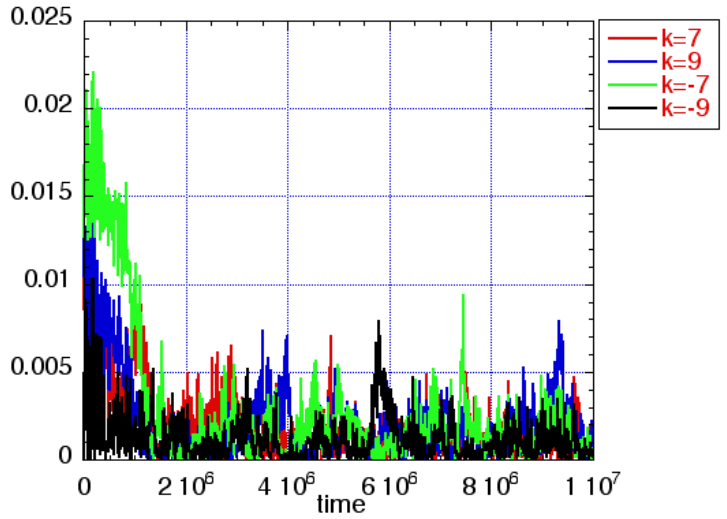
- Umklapp scattering is allowed, that is $k_1 \pm k_2 \pm .... \pm k_n \overset{N}{=} 0$
- in α-FPUT the 3-wave resonant manifold is empty
- via a canonical transformation, the 4-wave resonant manifold is not empty, but formed by isolated quartets!
- via a canonical transformation, the 6-wave resonant manifold is not empty and connected
- hence $t_{eq} \sim 1/\epsilon^8$, where the nonlinearity parameter is given by the initial condition



4-waves and thermalisation time-scales [PNAS 2015]



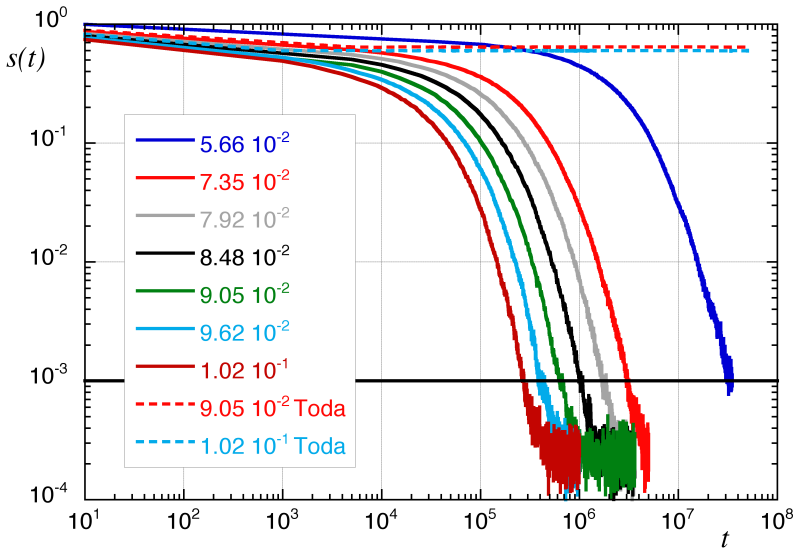
Here $\epsilon = 0.012$ and 3 modes belonging to the same quartet are initially excited: $k_1 = 7$, $k_2 = 9$, $k_3 = -7$.



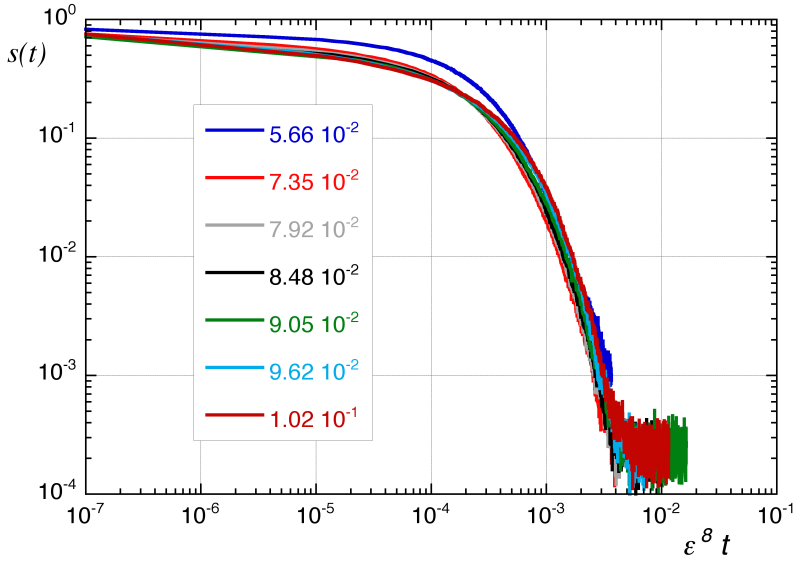
Here $\epsilon = 0.012$ and 3 modes belonging to the same quartet are initially excited: $k_1 = 7$, $k_2 = 9$, $k_3 = -7$.

Entropy measure and $t_{eq} \sim 1/\epsilon^8$ [PNAS 2015]

$$s(t) = \sum_k f_k \log f_k \quad \text{with} \quad f_k = \frac{N-1}{E_{tot}} \omega_k \langle |a_k|^2 \rangle, \quad E_{tot} = \sum_k \omega_k \langle |a_k|^2 \rangle$$



Entropy evolution for different nonlinearities ϵ vs. time t

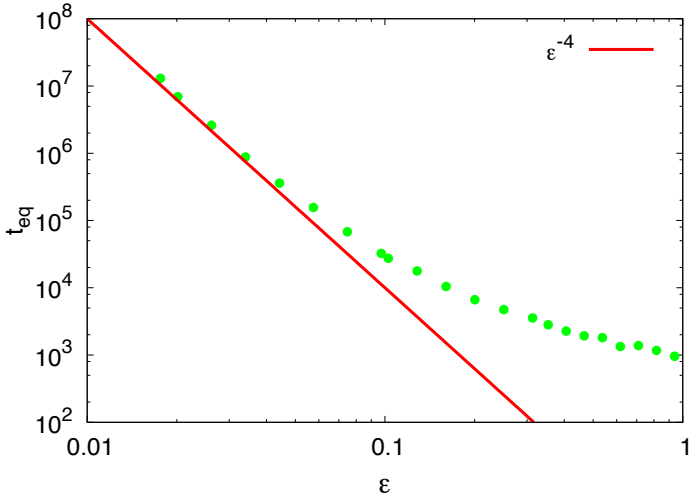


Entropy evolution for different nonlinearities ϵ vs. rescaled time $\epsilon^8 t$

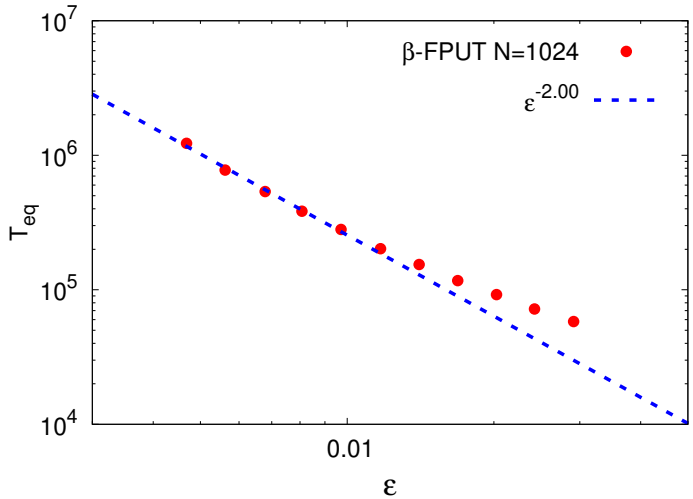
(averaging 1,000 realisations with initial conditions having the same wave mode amplitudes but phases uniformly distributed)

t_{eq} towards the thermodynamic limit $N \to \infty$

- All the previous reasoning and results are valid for small N (in our calculations $N = 64$)
- For large N, going towards the thermodynamic limit, the nonlinear broadening of the dispersion relation is large enough to let energy spreading between the isolated quartets, leading to for $t_{eq} \sim 1/\epsilon^4$
- This behaviour has been thoroughly investigated in the β-FPUT where $t_{eq} \sim 1/\epsilon^4$ for small N and $t_{eq} \sim 1/\epsilon^2$ for large N

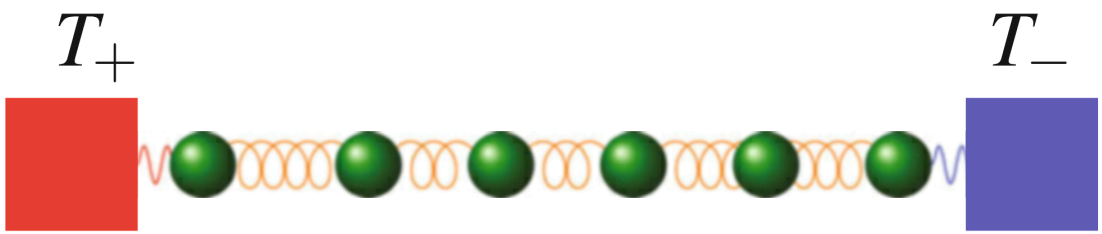


L'vov & Onorato (PRL 2018)



Pistone, et al. (MINE 2019)

The non-homogeneous problem



- Micro-scale: Newton's law, $m\ddot{\mathbf{x}}_i = -\nabla_i U$
- Meso-scale: wave kinetic equation, $\frac{\partial n_k}{\partial t} + v_k \frac{\partial n_k}{\partial x} = C(n_k)$ from WT
- Macro-scale: Fourier's law, $\mathbf{J} = -\kappa_e \nabla T$, where κ_e is the thermal conductivity

At macro-scale, applying the conservation law for energy (in 1-d)

$$\frac{\partial E}{\partial t} + \frac{\partial J}{\partial x} = 0 \quad \Longrightarrow \quad \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\kappa_e}{c}\frac{\partial T}{\partial x}\right]$$

where E is an energy per unit volume, $c = \partial E/\partial T$ the heat capacity
The temperature profile between two thermostats in stationary conditions, for constant κ_e/c, is $T(x) = ax + b$, that is linear

Anomalous conductivity/transport

In principle the conductivity (like the resistivity) is an intrinsic property of the material and should not depend on the size, however results emerged from intensive numerical simulations and experiments in low-dimensional systems show that:

- the conductivity may be size-dependent $\kappa_e(L) \sim L^\alpha$ where

$$\alpha = 0\,, \quad \text{normal conduction}$$
$$0 < \alpha \leq 1\,, \quad \text{anomalous conduction}$$
$$\alpha = 1\,, \quad \text{ballistic conduction}$$

- energy perturbations may propagate super-diffusively: a local perturbation of the energy broadens and its variance grows in time as

$$\sigma^2(t) \sim t^\beta\,, \quad \text{with} \qquad \beta > 1$$

Numerical and experimental evidence

Numerics: one-dimensional chain (Lepri, LNP 2016)

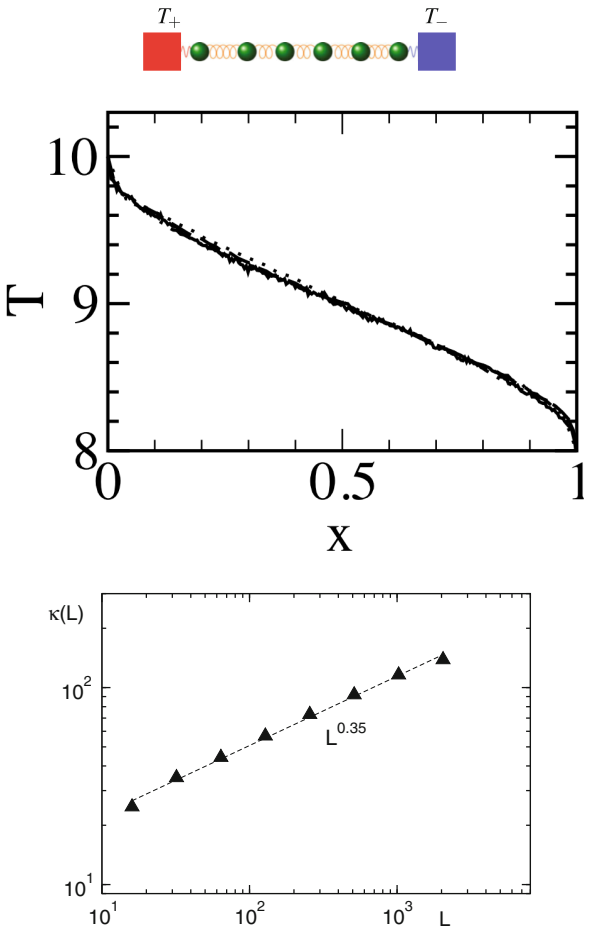


Fig. 1.3 Scaling of the finite-size conductivity for the FPU-$\alpha\beta$ model: with energy $e = 1$ and cubic coupling constant $\alpha = 0.1$

Experiments: SiGe nanowires (from C.W. Chang, 2016)

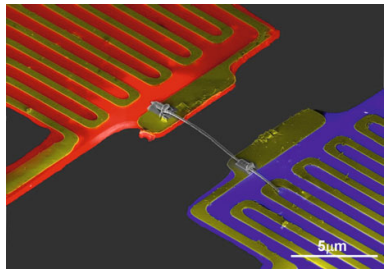
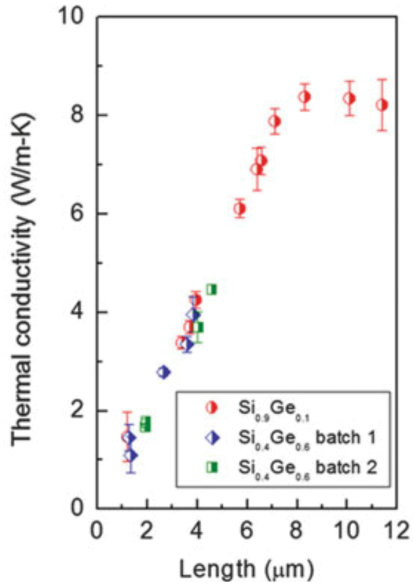


Fig. 8.5 A false colored SEM image of a thermal conductivity test fixture consisting of suspended heater and sensor pads with a SiGe nanowire anchored on it



The β-FPUT model with thermostats

$$\dot{q}_n = p_n$$
$$\dot{p}_n = (q_{n+1} + q_{n-1} - 2q_n) + \beta\left[(q_{n+1}) - q_n\right)^3 + (q_n - q_{n-1})^3\Big] - B(p_1, p_N)$$

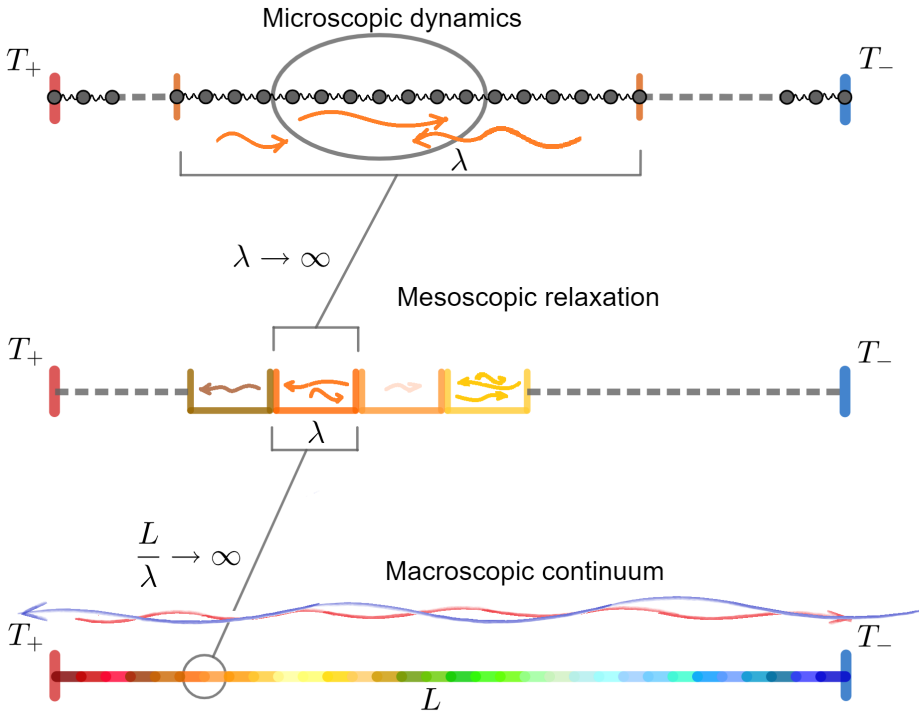
with

$$B(p_1, p_N) = \xi_1 p_1 \delta_{1,n} + \xi_N p_N \delta_{N,n}$$

where ξ_1 and ξ_N are Nosé-Hoover thermostats satisfying

$$\dot{\xi}_1 = \frac{1}{\tau_+^2}\left(\frac{p_1^2}{T_+} - 1\right)$$
$$\dot{\xi}_N = \frac{1}{\tau_-^2}\left(\frac{p_N^2}{T_-} - 1\right)$$

Understanding anomalous conduction [PRL 2020]

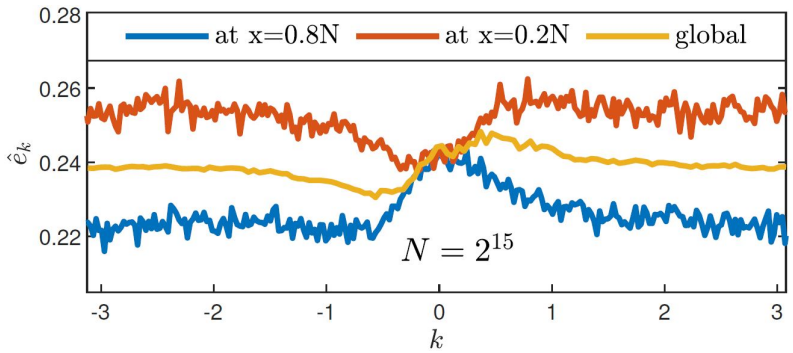


- A stationary state is reached when a net heat current flows through the lattice
- We assume the separation of scales $\lambda = \sqrt{L} \sim \sqrt{N}$ and measure "local" statistical properties averaging over the meso-scale λ

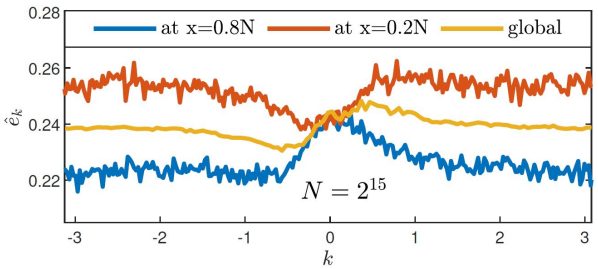
We compute the "local" wave energy spectral density

$$\hat{e}_k(k, x, t) = \omega_k \langle n_k(k, x, t) \rangle_\lambda \,,$$

where $n_k(k, x, t)$ is the wave spectral density



Symmetric part of the energy spectra [PRL 2020]



To highlight the asymmetry and behaviour around $k = 0$, we evaluate the symmetric part of the energy spectra

$$\frac{\hat{e}_k + \hat{e}_{-k}}{2},$$

where

$$\hat{e}_k(k, x, t) = \omega_k \langle n_k(k, x, t) \rangle_\lambda$$

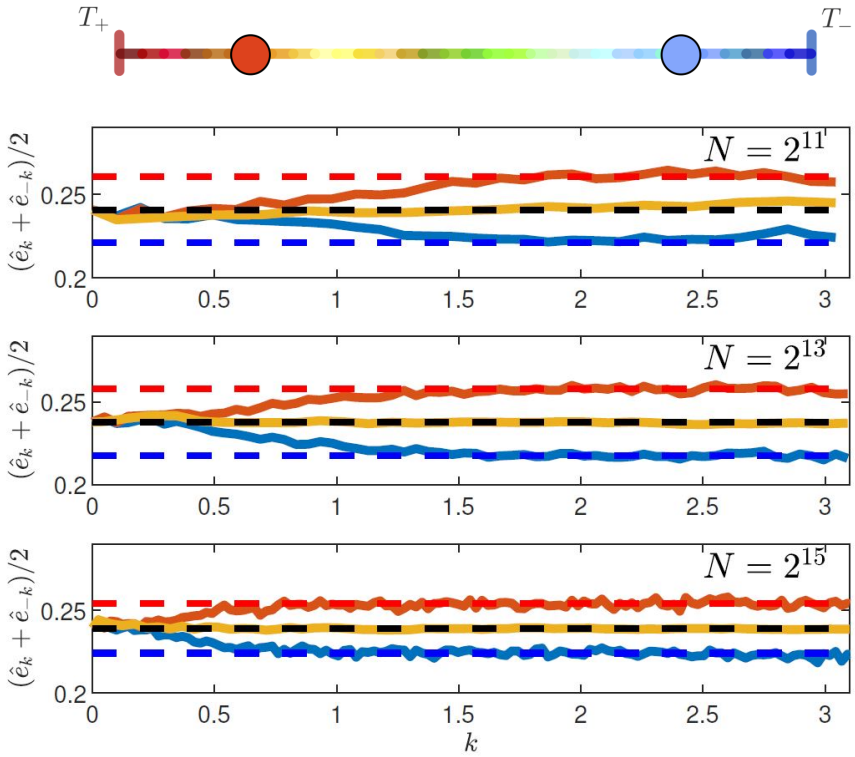
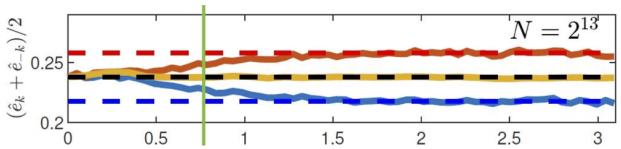


FIG. 2. The red and blue solid lines are the symmetrized stationary local energy spectra computed in windows of width $\sqrt{N}$ centered at $x_1 = 0.2N$ and $x_2 = 0.8N$, respectively. The dashed lines with same colors are at the respective average energy per particle at x_1 and x_2. The yellow line is the spectrum performed on the full chain.

Energy profile in space with decomposition [PRL 2020]



Introducing a cut-off scale k_c, we compute the total "local" energy as

$$e(x) = e^{>}(x; k_c) + e^{<}(x; k_c)\,,$$

where for $e^{>}$ only contributions from the modes with $|k| > k_c$ have been retained, and viceversa for $e^{<}$

The anomalous conduction results from the coexistence of ballistic modes and diffusive (kinetic) modes!

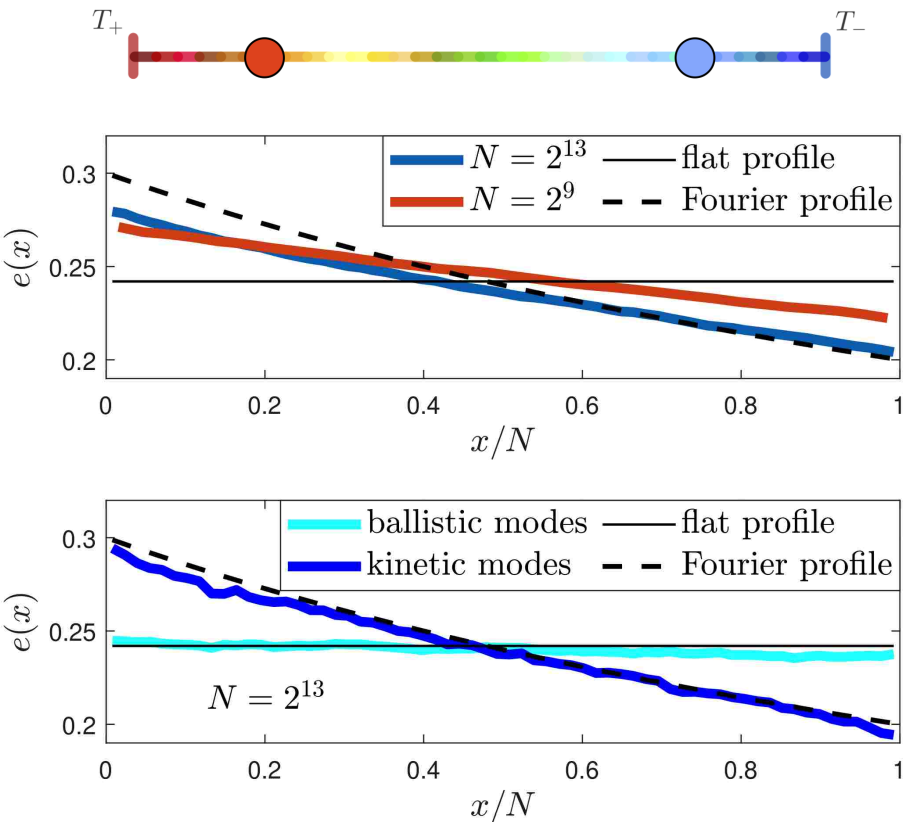


FIG. 3. Top: Numerical profiles of $e(x)$. Bottom: The blue line of the upper panel ($N = 2^{13}$) is decomposed into its contributions from $|k| \leq k_c$ (light blue) and $|k| > k_c$ (dark blue), normalized by the fraction of modes in each set: k_c/π and $(\pi - k_c)/\pi$, respectively. A value $k_c = 0.75$ is used, based on numerical estimate from Fig. 2.

Estimation of k_c [PRL 2020]

- assume 4-wave kinetic equation at meso-scale λ, that is

$$\frac{\partial n_k}{\partial t} + v_k \frac{\partial n_k}{\partial x} = C(n_k)\,, \quad \text{where } v_k = \frac{\partial \omega}{\partial k}$$

- In stationary conditions transport and collision integral contributions in the kinetic equation balance each other

$$\frac{v_{k_c}}{\lambda} \sim \frac{1}{\tau_{k_c}}$$

- Assuming small deviations from local equilibrium and small ks, a direct analytical calculation yields

$$\tau_k \sim k^{-5/3}\,, \quad \text{for} \quad |k| \ll 1 \quad \Longrightarrow \quad k_c \sim \lambda^{-3/5} \sim L^{-3/10}$$

Conclusions

- For small N the FPUT model exhibits a very long thermalisation time due to the (almost) absence of interactions between the modes of the system ($t_{eq} \propto 1/\epsilon^8$ for α-FPUT, $t_{eq} \propto 1/\epsilon^4$ for β-FPUT)
- for large N the nonlinear broadening is large enough and the effective KE has 4-wave interactions, where still long waves almost do not interact if the system is finite
- a separation of ballistic and diffusive scales, confirmed in deterministic simulations of β-FPUT by averaging over a mesoscale $\lambda \propto \sqrt{N}$, explains the anomalous diffusion without the need to invoke super-diffusion
- the separation scale can be estimated as $k_c \sim \lambda^{-3/5} \sim L^{-3/10}$ using the non-homogenous 4-wave KE

Outlooks

- analysis of the anomalous conduction as a superposition of ballistic and diffusive modes in the meso-scopic framework [work in progress!]
- accurate characterisation of the transport properties vs. temperature (and other eventual conserved quantities)
- derivation of the macroscopic model without fractional diffusion

Thanks for your attention!

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